

## II.G.8 Photoelectrochemical Hydrogen Production

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### Subcontractors:

- University of Hawaii at Manoa, Honolulu, HI
- Intematix Corporation, Fremont, CA
- Southwest Research Institute, San Antonio, TX
- Duquesne University, Pittsburgh, PA

Start Date: to be determined

Projected End Date: to be determined

(AC) Device Configuration Design

(AD) Systems Design and Evaluation

### Technical Targets

The core of this project comprises fundamental materials and device studies related to the development of multi-junction thin-film devices, such as the “Hybrid Photoelectrode” (HPE), for PEC hydrogen production. Insights gained from these studies will be applied toward the design and manufacture of PEC hydrogen-production systems that meet the DOE 2013 production targets in efficiency, durability and, ultimately, cost. Specific goals toward reaching the longer-term targets include:

- Development of new, low-cost photoactive materials with 1-sun photocurrents greater than 6 mA/cm<sup>2</sup> and with sufficient durability to meet the lifetime requirement.
- Development of supporting solid-state devices with sufficient current and voltage output.
- Development of necessary process integration techniques.
- Demonstration of materials/device fabrication process scale-up for commercialization.
- Generation of an energy/economic analysis for hydrogen production cost based on the developed technology.

### Objectives

- The demonstration of a multi-junction photoelectrochemical (PEC) solar-powered hydrogen production system with 8% solar-to-hydrogen (STH) conversion efficiency and 1,000 hours operational life, consistent with the DOE 2013 targets.
- The identification of commercialization paths toward DOE plant production cost targets.

### Technical Barriers

This project addresses the following technical barriers from the Photoelectrochemical Hydrogen Production from Water section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

- (Y) Materials Efficiency
- (Z) Materials Durability
- (AA) PEC Device and Auxiliary Material
- (AB) Bulk Materials Synthesis

### Accomplishments

Funding has not started for this project; therefore there is no technical progress to report. However, some important accomplishments include:

- Establishment of the technical research team with specification of team-member roles in the development high-performance PEC materials using state-of-the-art theoretical, synthesis and characterization techniques.
- Identification of further important collaborative opportunities with the National Renewable Energy Laboratory (NREL), with members of the University of Nevada, Las Vegas (UNLV) Solar Hydrogen Generation Research (SHGR) PEC team, and others for facilitating this research.
- Establishment of PEC focus materials classes, including tungsten-based compounds, silicon-based compounds, copper-chalcopyrite based compounds (and others), as the primary basis for the materials research and development effort.



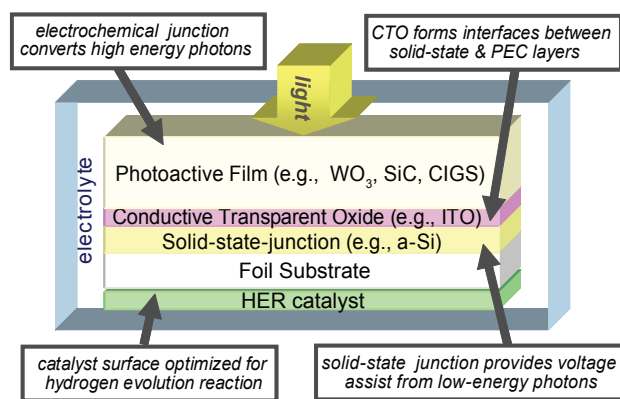
## Introduction

This research project focuses on the development of practical PEC water splitting systems for hydrogen production based on multi-junction thin-film semiconductor devices, such as the University of Hawaii (UH) – patented hybrid photoelectrode (HPE), illustrated in Figure 1. HPE technology is based on low-cost materials such as metal foil substrates, and incorporates thin-film photovoltaic (PV) films (such as amorphous silicon) and PEC films (such as metal-oxides) in multi-junction device configurations capable of efficiently splitting water. The identification of scalable fabrication processes for commercial-scale systems is also a key emphasis.

## Approach

In order to develop efficient and cost-effective HPE systems, new photoactive PEC material films with improved photo-current, photo-voltage, and durability properties need to be identified and developed. In conjunction, auxiliary materials and components will need to be developed for incorporation, with the best developed PEC films, in effective HPE device designs. Specific research and development areas within this integrated materials/device approach include:

- Accelerated Research and Development of Photoactive Materials
  - Advanced synthesis and screening of PEC materials
  - Doping for improved photo-response
  - Film modification for improved interfaces
  - Guidance by theoretical materials models
  - Guidance through detailed characterization of existing high-performance materials
- Hybrid Photoelectrode Device Development
  - Development of suitable solid-state junctions for device integration
  - Prototype demonstration based on best-available materials
- Scale-up and Commercialization Evaluation
  - Mid-scale fabrication of HPE component films using cluster tool technology
  - Identification of pathways to large-scale fabrication
  - Economic/energy analysis of HPE technology based on current state and projections



**FIGURE 1.** The Hybrid Photoelectrode Structure Showing the Function of Constituent Thin Film Layers

## Results

Funding has not started for this project; therefore there is no technical progress to report. However, there have been a number of important accomplishments in terms of building and re-defining the research emphases and the research team, and in establishing promising focus PEC materials. Recent collaborative work with the UNLV SHGR-PEC program (including a range of participating research organizations such as NREL, the University of Hawaii, the University of California, Santa Barbara, and others), has helped expand the scope of the PEC materials R&D in terms of state-of-the-art theory, synthesis and characterization capabilities. In addition, a group of focus PEC materials classes has been identified with the most promise for incorporation in efficient and durable multi-junction water-splitting devices, including tungsten-based compounds, silicon-based compounds, and copper-chalcopryrite-based compounds (consistent with the scope of this project), as well as iron-based compounds, titanium-based compounds, zinc-based compounds (and others) which are being developed by the DOE in complementary research projects.

## Conclusions and Future Directions

With the advent of funding, the preparatory work in establishing materials research collaborations in areas of theory, synthesis and characterization, and in establishing focus PEC materials classes will become an invaluable platform for launching a well-focused DOE research project to develop effective PEC hydrogen production systems. Working closely with DOE and with other DOE-sponsored research groups is expected to greatly expedite successful breakthroughs and results in this area.